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Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 324 °C

Global applicability domain: Outside

Local applicability domain index: 1.15e-01

Confidence level: 6.89e-01

Nearest Neighbors from the Training Set

Image not found
Ametryn
Measured: 345
Predicted: 341

Image not found
Desmetryn
Measured: 345
Predicted: 341

Image not found
Tetraethylenepentamine
Measured: 342
Predicted: 339

Image not found
2-Pyridinamine, N-2-pyridinyl-
Measured: 308
Predicted: 322

Image not found
Triethylenetetramine
Measured: 267
Predicted: 265